

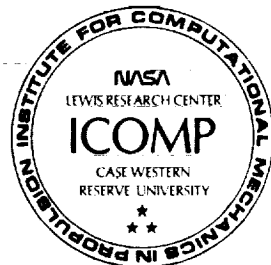
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On the Application of Subcell Resolution to Conservation Laws With Stiff Source Terms

Shih-Hung Chang
Cleveland State University
Cleveland, Ohio

and Institute for Computational Mechanics in Propulsion
Lewis Research Center
Cleveland, Ohio

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ON THE APPLICATION OF SUBCELL RESOLUTION TO CONSERVATION LAWS WITH STIFF SOURCE TERMS

Shih-Hung Chang*
Department of Mathematics
Cleveland State University
Cleveland, Ohio 44115

and Institute for Computational Mechanics in Propulsion
Lewis Research Center
Cleveland, Ohio 44135

ABSTRACT

LeVeque and Yee recently investigated a one-dimensional scalar conservation law with stiff source terms modeling the reacting flow problems and discovered that for the very stiff case most of the current finite difference methods developed for non-reacting flows would produce wrong solutions when there is a propagating discontinuity. A numerical scheme, ENO/SRCD_A, is proposed in this report for solving conservation laws with stiff source terms. This scheme is a modification of Harten's ENO scheme with subcell resolution, ENO/SR. The locations of the discontinuities and the characteristic directions are essential in the design. Strang's time-splitting method is used and time evolutions are done by advancing along the characteristics. Numerical experiment using this scheme shows excellent results on the model problem of LeVeque and Yee. Comparisons of the results of ENO, ENO/SR, and ENO/SRCD are also presented.

(...) *subcell resolution*

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1. INTRODUCTION

In the investigation of numerical methods for reacting flow problems, LeVeque and Yee [4] recently considered certain fundamental questions concerning the quality of numerical solutions. Namely, in extending current finite difference techniques developed for non-reacting flows to reacting flows, can one: (i) develop stable methods, (ii) obtain "high resolution" results with sharp discontinuities and second order accuracy in smooth regions, and (iii) obtain the correct jumps at the correct locations? They introduced and studied the following one-dimensional scalar conservation law with parameter-dependent source term

$$u_t + u_x = \psi(u), \quad (1)$$

$$\psi(u) = -\mu u \left(u - \frac{1}{2}\right) (u - 1), \quad (2)$$

where μ is a parameter. This equation becomes stiff when the parameter μ is large. Although this linear advection equation with a source term represents only a simple model of reacting flow problems, by studying the numerical solutions one encounters some of the intriguing difficulties sure to occur in solving more realistic models.

In their study, two different approaches were used to construct second order accurate numerical methods. One approach was to use a modification of MacCormack's predictor-corrector method for conservation laws, together with two TVD-like versions with appropriate limiters. The other approach was based on the second order accurate Strang splitting method [5]. Their numerical tests revealed that stable and second order schemes can be devised by using either of these approaches. However, in studying the ability of these methods in dealing with propagating discontinuities, it was reported that for a fixed mesh and for the very stiff case, all the methods produced solutions that look reasonable and yet are completely wrong, because the discontinuities are in the wrong locations. Their investigation pointed out that the main difficulty is the smearing of the discontinuity in the spatial direction, which in turn introduced a nonequilibrium state into the calculation. To avoid this difficulty, it will be necessary to increase the resolution near the discontinuity, at least for the purpose of evaluating $\psi(u)$.

Integrating Eq. (1) over $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}] \times [t_n, t_{n+1}]$, one obtains

$$\begin{aligned} \bar{u}_j^{n+1} = \bar{u}_j^n - \frac{1}{\Delta x} \left[\int_{t_n}^{t_{n+1}} u(x_{j+\frac{1}{2}}, t) dt - \int_{t_n}^{t_{n+1}} u(x_{j-\frac{1}{2}}, t) dt \right] \\ + \frac{1}{\Delta x} \int_{t_n}^{t_{n+1}} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \psi(u(x, t)) dx dt, \end{aligned} \quad (3)$$

where \bar{u}_j^n denotes the cell average of u over $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ at t_n . From this integral equation formulation, one can see that a source of error is also from the evaluation of the double integral term in (3). Because in most numerical methods the function

$\psi(u)$ is replaced by ψ evaluated at a fixed value of u . This may produce a reasonable approximation only when u is smooth.

The purpose of this paper is to show that numerical methods can be devised to overcome the above mentioned difficulties. We will construct a numerical scheme which, when applied to Eq. (1), results in stable solutions with excellent resolutions at the correct locations of the discontinuities. Essential to the construction of this scheme is the application of Harten's ENO reconstruction with subcell resolution [2]. The subcell resolution is an idea based on the observation that unlike point values, cell averages of a discontinuous piecewise smooth function contain information about the exact location of the discontinuity within the cell. Using this observation in his study of conservation laws, Harten [2] proposed reconstruction techniques and obtained modifications of the ENO schemes [3] showing significant improvement in the resolution of contact discontinuities. Basically, when good approximations to the exact locations of the discontinuities inside the cells can be obtained, it is then possible to have good reconstruction of the solution at each time step. Here we will also demonstrate that when the information on the location of the discontinuity is used in treating the source term, the results will improve significantly.

To maintain second order accuracy, we will use the approach of Strang's time-splitting method [5] in which one alternates between solving the conservation law without the source term and the ordinary differential equation modeling the chemistry. The numerical solution v^{n+1} at time step t_{n+1} is computed from v^n by

$$v^{n+1} = S_\psi\left(\frac{\Delta t}{2}\right) S_f(\Delta t) S_\psi\left(\frac{\Delta t}{2}\right) v^n. \quad (4)$$

where $S_f(\Delta t)$ represents the numerical solution operator for the conservation law without the source term over a time step Δt , and $S_\psi\left(\frac{\Delta t}{2}\right)$ represents the numerical solution operator for the ordinary differential equation

$$u_t = \psi(u), \quad (5)$$

over $\Delta t/2$. In terms of the integral equation formulation (3), S_f takes care of the flux terms represented by the two single integrals at $x_{j\pm\frac{1}{2}}$, and S_ψ handles the double integral term.

We will outline the construction of the two operators S_f and S_ψ in section 2, which depends on the characteristic directions as well as the ENO reconstruction with subcell resolution procedure [2]. For the purpose of comparison, we will also test numerical schemes which use a ENO and a ENO with subcell resolution as S_f . These algorithms will also be stated briefly in section 2. In section 3, we report the numerical results obtained from using the above schemes on the same model problem of LeVeque and Yee [4]. A conclusion will be given in section 4.

2. CONSTRUCTION OF THE SCHEMES

We first describe the structure of the operator $S_f(\Delta t)$. At the time step t_n , suppose that we have obtained the numerical solution $v^n = \{v_j^n\}$, where v_j^n represents an

approximation to the cell average \bar{u}_j^n . Then, to obtain $S_f(\Delta t) v^n$, we use the following steps:

1. Obtain a reconstruction $R(x; v^n)$ from the given values v^n .
2. Modify this reconstruction $R(x; v^n)$ to obtain $\hat{R}(x; v^n)$ using the subcell resolution when discontinuity is detected.
3. Advance $\hat{R}(x; v^n)$ along the characteristics from t_n to t_{n+1} and then take cell averages to complete $S_f(\Delta t) v^n$.

In the scheme we propose, the steps 1 and 2 will follow the basic ENO reconstruction procedure with subcell resolution of Harten [2]. The reconstructed solution function $R(x; v^n)$ here is a piecewise quadratic polynomial obtained by using the primitive function approach. For the sake of completeness, we will describe in straightforward terms the procedures used. For more details and general discussions on reconstruction and subcell resolution, see Harten [2].

Step 1. ENO Reconstruction

Over each cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, choose $i = i(j)$ such that

$$|v_{i+2}^n - 2v_{i+1}^n + v_i^n| = \min \{|v_{k+2}^n - 2v_{k+1}^n + v_k^n| : k = j-2, j-1, j\}.$$

Let $R_j(x; v^n)$ denote the reconstructed quadratic polynomial over this cell. Then

$$R_j(x; v^n) = a_j + s_j (x - x_j) + \frac{1}{2} c_j (x - x_j)^2, \quad (6)$$

where

$$\begin{aligned} c_j &= (v_{i+2}^n - 2v_{i+1}^n + v_i^n) / (\Delta x)^2, \\ s_j &= (v_{i+1}^n - v_i^n) / \Delta x + (j - i - \frac{1}{2}) c_j \Delta x, \\ a_j &= v_j^n - c_j (\Delta x)^2 / 24. \end{aligned} \quad (7)$$

Step 2. Subcell Resolution

To detect a discontinuity in a cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, we define

$$F_j(z) = \frac{1}{\Delta x} \left[\int_{x_{j-\frac{1}{2}}}^z R_{j-1}(x; v^n) dx + \int_z^{x_{j+\frac{1}{2}}} R_{j+1}(x; v^n) dx \right] - v_j^n. \quad (8)$$

In the schemes we tested, the following criterion is used. If

$$|s_j| > |s_{j-1}|, |s_j| > |s_{j+1}|, \quad \text{and} \quad F_j(x_{j-\frac{1}{2}}) F_j(x_{j+\frac{1}{2}}) \leq 0, \quad (9)$$

we consider that there is a discontinuity at θ_j in this cell satisfying

$$F_j(\theta_j) = 0. \quad (10)$$

The location θ_j can be approximated by using any standard root-finding method. We simply use the bisection method in our experiment.

Now, if there is a discontinuity inside the cell, a modified reconstruction $\hat{R}_j(x; v^n)$ is used, where

$$\hat{R}_j(x; v^n) = \begin{cases} R_{j-1}(x; v^n), & x_{j-\frac{1}{2}} \leq x < \theta_j, \\ R_{j+1}(x; v^n), & \theta_j < x \leq x_{j+\frac{1}{2}}. \end{cases}$$

Otherwise, we use

$$\hat{R}_j(x; v^n) = R_j(x; v^n).$$

Step 3. Time Evolution and Cell Averaging

Here we choose to describe the scheme for the conservation law

$$u_t + a u_x = 0, \quad a > 0. \quad (11)$$

It can be handled similarly for $a < 0$. Consider the case $a \Delta t \leq \Delta x$ and that there exists a discontinuity at θ_j inside the cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ with

$$\theta_j \leq x_{j+\frac{1}{2}} - a \Delta t,$$

as shown in Fig. 1. The idea is that, following the characteristics from t_n to t_{n+1} , we will find an approximation to

$$S_f(\Delta t) v_j^n = \frac{1}{\Delta x} \left[\int_{x_{j-\frac{1}{2}} - a \Delta t}^{\theta_j} R_{j-1}(x; v^n) dx + \int_{\theta_j}^{x_{j+\frac{1}{2}} - a \Delta t} R_{j+1}(x; v^n) dx \right]. \quad (12)$$

In our present scheme we use the following simple computation. Let x_m and x_p denote the midpoints in the intervals $(x_{j-\frac{1}{2}} - a \Delta t, \theta_j)$ and $(\theta_j, x_{j+\frac{1}{2}} - a \Delta t)$ respectively (see Fig. 1). Then compute

$$\begin{aligned} S_f(\Delta t) v_j^n &= [R_{j-1}(x_m; v^n) (\theta_j - x_{j-\frac{1}{2}} + a \Delta t) \\ &\quad + R_{j+1}(x_p; v^n) (x_{j+\frac{1}{2}} - a \Delta t - \theta_j)] / \Delta x. \end{aligned} \quad (13)$$

Other locations of θ_j and the cases with smooth regions can be treated similarly and easily. It is quite simple to modify the above scheme for more general equations and also to write higher order versions of it.

Now, let us describe the operator $S_\psi(\Delta t)$. It is essentially the approximation of the double integral term in Eq.(3). Let us use the same notations introduced above and refer to Fig. 1. To advance the value $R_{j-1}(x_m; v^n)$ from t_n to t_{n+1} , we again follow the characteristics to obtain an approximate value

$$R_{j-1}(x_m; v^n) + \Delta t \psi(R_{j-1}(x_m; v^n)),$$

using the simple Euler's method. Let z_m and z_p denote the midpoints in the intervals $(x_{j-\frac{1}{2}}, \theta_j)$ and $(\theta_j, x_{j+\frac{1}{2}})$ respectively. Then, for the case $a > 0$ and $\theta_j \leq x_{j+\frac{1}{2}} - a \Delta t$, we use

$$\begin{aligned} S_\psi(\Delta t) v_j^n = & v_j^n + \frac{\Delta t}{2 \Delta x} [\psi(R_{j-1}(z_m; v^n)) (\theta_j - x_{j-\frac{1}{2}}) \\ & + \psi(R_{j-1}(x_m; v^n) + \Delta t \psi(R_{j-1}(x_m; v^n))) (\theta_j - x_{j-\frac{1}{2}} + a \Delta t) \\ & + \psi(R_{j+1}(z_p; v^n)) (x_{j+\frac{1}{2}} - \theta_j) \\ & + \psi(R_{j+1}(x_p; v^n) + \Delta t \psi(R_{j+1}(x_p; v^n))) (x_{j+\frac{1}{2}} - \theta_j - a \Delta t)]. \end{aligned} \quad (14)$$

Again, other situations are handled similarly.

The resulting algorithm then takes the following form:

$$v_j^{n+1} = S_\psi\left(\frac{\Delta t}{2}\right) S_f(\Delta t) S_\psi\left(\frac{\Delta t}{2}\right) v_j^n. \quad (15)$$

Two things are essential in the design of the above algorithm, namely, the location of the discontinuity θ_j and the characteristic direction. We approximate θ_j by following the ENO reconstruction with subcell resolution procedure. For this reason, we denote this algorithm by ENO/SRCD. In applying this algorithm to Eq. (1), one takes the value $a = 1$. In treating more general equations, the formulas in step 3 can be easily modified.

For the purpose of comparison, we have tested several other schemes. We shall report the results from using a ENO scheme and also a ENO scheme with subcell resolution, ENO/SR, of Harten [2] as the operator $S_f(\Delta t)$. The following version of the ENO scheme has been used in [1].

ENO Scheme:

For the operator $S_f(\Delta t)$, we use

$$S_f(\Delta t) v_j^n = v_j^n - \frac{\Delta t}{\Delta x} (\bar{f}_{j+\frac{1}{2}} - \bar{f}_{j-\frac{1}{2}}), \quad (16)$$

where

$$\begin{aligned} \bar{f}_{j+\frac{1}{2}} = \bar{f}_{j+\frac{1}{2}}^{ENO} = & \frac{1}{2} [f^R(\tilde{v}_j(x_{j+\frac{1}{2}}, t_n), \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_n)) \\ & + f^R(\tilde{v}_j(x_{j+\frac{1}{2}}, t_{n+1}), \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_{n+1}))], \end{aligned} \quad (17)$$

with

$$\begin{aligned} \tilde{v}_j(x_{j+\frac{1}{2}}, t_n) &= v_j^n + \frac{\Delta x}{2} s_j, \\ \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_n) &= v_{j+1}^n - \frac{\Delta x}{2} s_{j+1}, \\ \tilde{v}_j(x_{j+\frac{1}{2}}, t_{n+1}) &= v_j^n + \frac{\Delta x}{2} s_j - \Delta t a s_j, \\ \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_{n+1}) &= v_{j+1}^n - \frac{\Delta x}{2} s_{j+1} - \Delta t a s_{j+1}, \end{aligned}$$

where the s_j 's used in the computation come from (7) in step 1, $a = 1$ for Eq.(1), and $f^R(v_L, v_R)$ denotes the flux at the origin in a Riemann problem with v_L to the left and v_R to the right.

In [2], there is a simpler version of second order ENO scheme. The difference is from the approximation of the two single integrals at $x_{j \pm \frac{1}{2}}$ in Eq.(3). The ENO in [2] uses a midpoint rule to do the approximation, while a trapezoidal rule is used in the above formulation. Since in our test Eq.(17) produces slightly better computational results, we choose to report it here. The operator $S_\psi(\Delta t)$ will be the same as in Eq.(14) and the final algorithm also takes the same form as in Eq.(15).

ENO/SR Scheme:

The operator $S_f(\Delta t)$ is now replaced by Harten's second order ENO scheme with subcell resolution [2]. The entire algorithm is denoted here also by ENO/SR. The construction of $S_f(\Delta t)$ is described again for Eq.(11) in the form of Eq.(16) with

$$\bar{f}_{j+\frac{1}{2}} = \bar{f}_{j+\frac{1}{2}}^{ENO} + \hat{g}_{j+\frac{1}{2}},$$

where $\bar{f}_{j+\frac{1}{2}}^{ENO}$ will be the same as in Eq.(17) and the correction term $\hat{g}_{j+\frac{1}{2}}$ is computed as follows. If the discontinuity condition (9) is not satisfied, then

$$\hat{g}_{j+\frac{1}{2}} = \frac{a}{12} (\nu - 1) (2\nu - 1) c_j (\Delta x)^2, \quad \nu = a \Delta t / \Delta x;$$

else

$$\hat{g}_{j+\frac{1}{2}} = \begin{cases} [(\Delta x - a \Delta t) (v_j^n - a \Delta t s_j / 2) - b_{j-1}(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}} - a \Delta t)] / \Delta t, & \text{when } F_j(x_{j+\frac{1}{2}} - a \Delta t) F_j(x_{j-\frac{1}{2}}) > 0, \\ [b_{j+1}(x_{j+\frac{1}{2}} - a \Delta t, x_{j+\frac{1}{2}}) - a \Delta t (v_j^n + (\Delta x - a \Delta t) s_j / 2)] / \Delta t, & \text{otherwise,} \end{cases}$$

and the expression $b_j(y_1, y_2)$ is used to mean

$$b_j(y_1, y_2) = \int_{y_1}^{y_2} R_j(x; v^n) dx.$$

In the above formulas, all the a_j 's, s_j 's, and c_j 's come from (7) in step 1. We also use the same operator $S_\psi(\Delta t)$ from (14) and the final algorithm again takes the formal form of (15).

3. COMPUTATIONAL RESULTS

We use the same mesh and initial data as in the model problem of LeVeque and Yee [4] to test the ability of the above schemes in dealing with propagating discontinuities. Thus Eq.(1) is solved together with the initial condition

$$u(x, 0) = \begin{cases} 1, & \text{if } x \leq 0.3, \\ 0, & \text{if } x > 0.3. \end{cases}$$

We take $\Delta x = 0.02$, $\Delta t = 0.015$, and the domain in x to be from 0 to 1. For comparison with [4], we also show the results at $t = 0.3$ and for the cases $\mu = 1, 10, 100$, and 1000. Figure 2 shows the computed results using the ENO, ENO/SR, and ENO/SRCD schemes for $\mu = 1, 10$, and 100. For the very stiff case, $\mu = 1000$, both ENO and ENO/SR schemes fail to produce stable solutions for the above mesh in our computational experiment. Only the ENO/SRCD scheme still produces excellent results as shown in Fig. 3. However, when we reduce the size of Δt to one half of the original, i.e., $\Delta t = 0.0075$, and march 40 time steps, excellent results are again obtained from both ENO and ENO/SR schemes as shown in Fig. 4. Of course, reducing Δt means the reduction of the stiffness of the system. The difficulty arises from the fact that in both the ENO and ENO/SR schemes, the computation of the numerical flux $\bar{f}_{j+\frac{1}{2}}^{ENO}$ still produces "large" error in the spatial direction.

The computational results obtained here compare favorably to those in LeVeque and Yee [4].

4. CONCLUSIONS

We have proposed a numerical scheme ENO/SRCD, which is a modification of Harten's ENO scheme with subcell resolution ENO/SR, for solving conservation laws with stiff source terms. We use Strang's time-splitting method and treat the conservation law without the source term and an ordinary differential equation with the source term representing the chemistry sequentially. For both the conservation law solution operator S_f and the ordinary differential equation solution operator S_ψ , the locations of the discontinuities and the characteristic directions are essential in their design. The main difference between the construction of this S_f and that of Harten's ENO/SR is that the time evolution here is accomplished by advancing along the characteristics explicitly, while ENO/SR uses the numerical flux $\bar{f}_{j+\frac{1}{2}}^{ENO}$ followed by a correction term based on the location of the discontinuity. The operator S_ψ for the ordinary differential equation also advances along the characteristics. Our numerical experiment using this scheme shows excellent results on the model problem of LeVeque and Yee [4] for reacting flows. Comparisons of the results of ENO, ENO/SR, and ENO/SRCD have also been presented.

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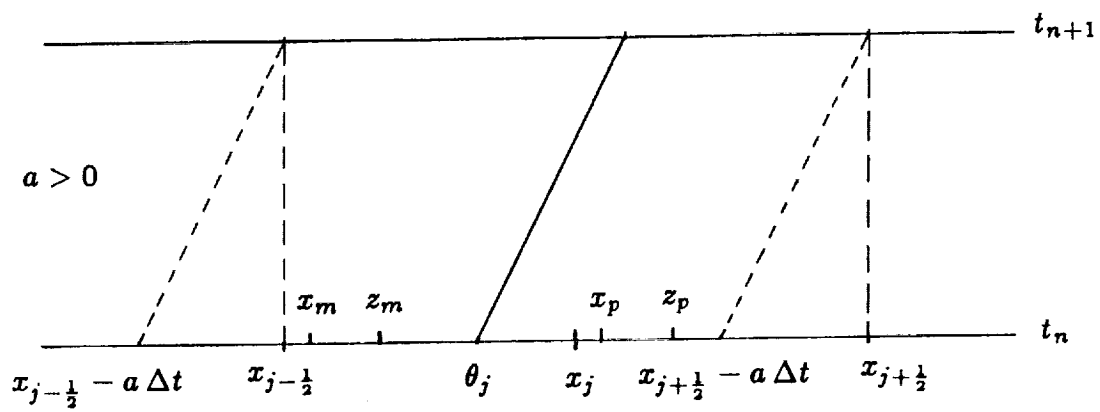


Fig. 1. The case $\theta_j \leq x_{j+\frac{1}{2}} - a\Delta t$

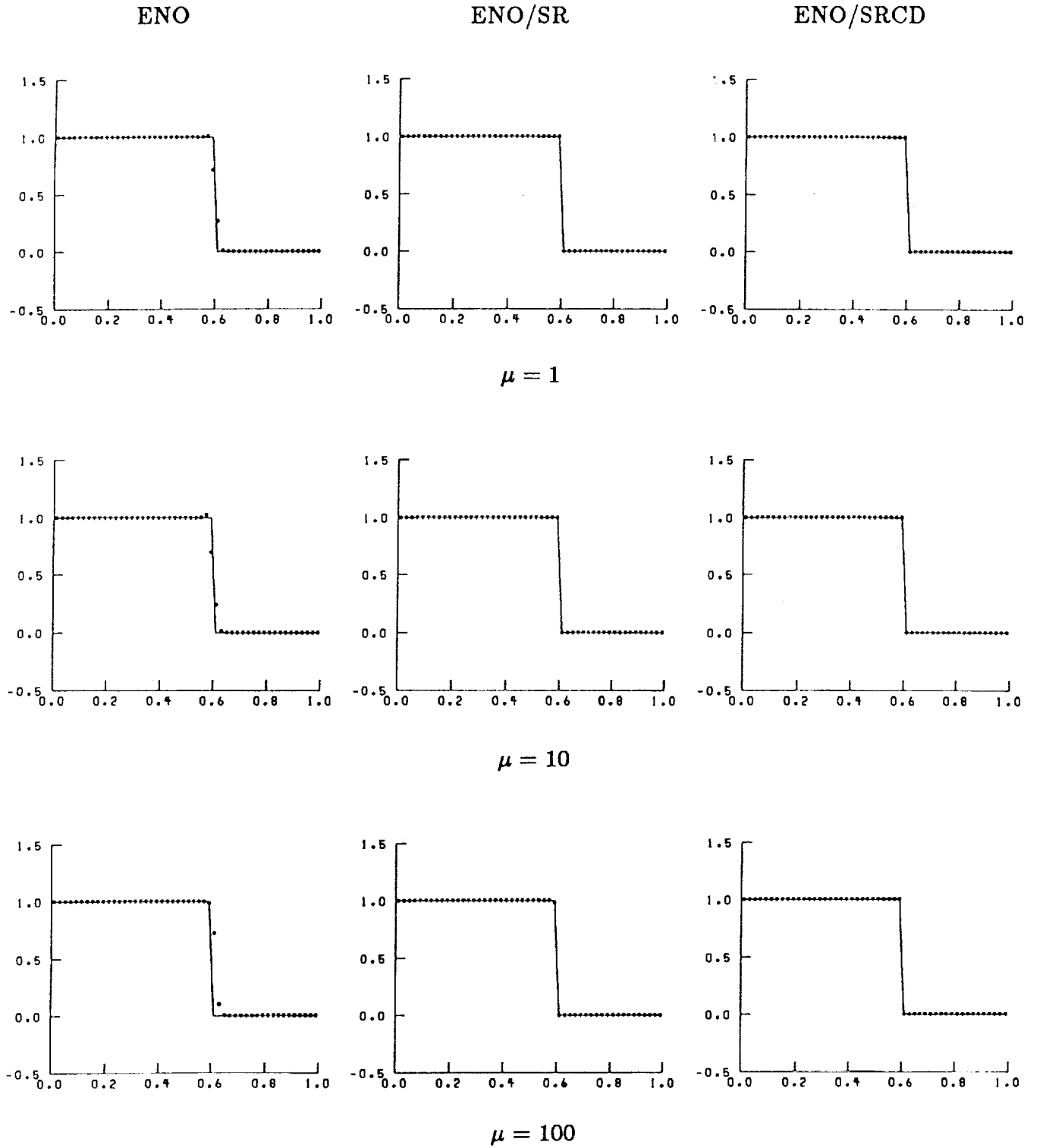


Fig. 2. Numerical results at $t = 0.3$ using ENO (first column), ENO/SR (second column), and ENO/SRCD (third column) schemes with discontinuous initial data for $\mu = 1$ (first row), $\mu = 10$ (second row), and $\mu = 100$ (third row). $\Delta x = 0.02$, $\Delta t = 0.015$, —: true solution, \cdots : computed solution

ENO/SRCD

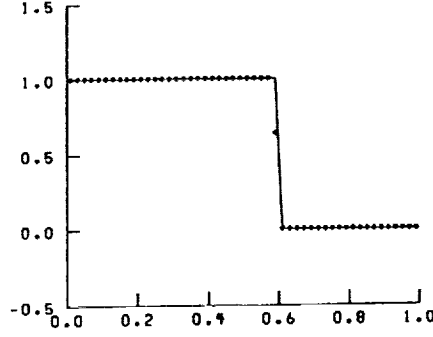
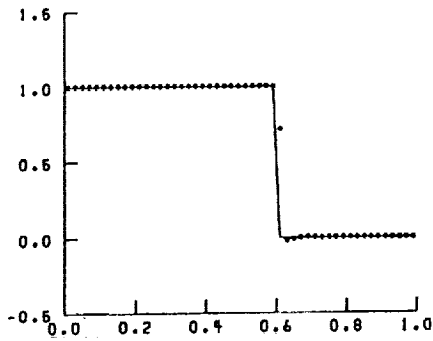


Fig. 3. Numerical results at $t = 0.3$ using ENO/SRCD scheme with discontinuous initial data and $\mu = 1000$.
 $\Delta x = 0.02$, $\Delta t = 0.015$, —: true solution, \cdots : computed solution

ENO



ENO/SR

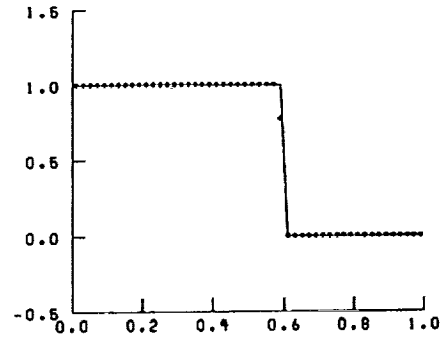


Fig. 4. Numerical results at $t = 0.3$ using ENO and ENO/SR schemes with discontinuous initial data and $\mu = 1000$.
 $\Delta x = 0.02$, $\Delta t = 0.0075$, —: true solution, \cdots : computed solution

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16. Abstract LeVeque and Yee recently investigated a one-dimensional scalar conservation law with stiff source terms modeling the reacting flow problems and discovered that for the very stiff case most of the current finite difference methods developed for non-reacting flows would produce wrong solutions when there is a propagating discontinuity. A numerical scheme, ENO/SRCD, is proposed in this report for solving conservation laws with stiff source terms. This scheme is a modification of Harten's ENO scheme with subcell resolution, ENO/SR. The locations of the discontinuities and the characteristic directions are essential in the design. Strang's time-splitting method is used and time evolutions are done by advancing along the characteristics. Numerical experiment using this scheme shows excellent results on the model problem of LeVeque and Yee. Comparisons of the results of ENO, ENO/SR, and ENO/SRCD are also presented.					
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